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Ab initio molecular dynamics

Potential energy surfaces (PES) generated by ab initio electronic structure calculations are best suited to perform molecular dynamics simulations on complex systems (e.g. ternary or quaternary alloys) or on systems undergoing physical processes such as electron transfer or chemical reactions. The price to pay is a dramatic increase of CPU time with respect to simulations based on empirical interatomic potentials. At the time being, ab initio molecular dynamics only allows to simulate relatively small systems (of a few hundreds of atoms) on relatively small time scales (a few picoseconds). This talk will present some recent techniques allowing to improve and accelerate ab initio molecular dynamics calculations.